

DERWENT-ACC-NO: 2000-283531

DERWENT-WEEK: 200651

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TITLE: New pyrrolo(2,3-d)pyrimidine derivatives,
useful for treatment of e.g. angiogenesis, vascular
permeability, immune response, inflammation, cancer and
respiratory disorders and to decrease fertility are protein
kinase inhibitors

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JOHNSTON, D N
; MAZDIYASNI, H ; MUNSCHAUER, R ; RAFFERTY, P ; TOMETZKI, G B ;
TWIGGER, H
L ; ARNOLD, D ; DENG, B ; JOHNSTON, N ; TOMETZKI, B ; TWIGGER, L
; JOHNSON, D N ; MUNSCHUER, R ; HIRST, G C ; ARNOLD, L ;
MAZDIYASNI, H H G

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PRIORITY-DATA: 1998US-100954P (September 18, 1998) , 1998US-0042702
(March 17,
1998) , 1999US-0399083 (September 17, 1999)

PATENT-FAMILY:

PUB-NO	MAIN-IPC	PUB-DATE	LANGUAGE
DE 69928414 T2		August 3, 2006	N/A
000	C07D 487/00		
*WO 200017202 A1		March 30, 2000	E
242	C07D 487/04		
AU 9960475 A		April 10, 2000	N/A
000	C07D 487/04		
NO 200101357 A		May 14, 2001	N/A
000	C07D 487/04		
EP 1114052 A1		July 11, 2001	E
000	C07D 487/04		
CZ 200100959 A3		December 12, 2001	N/A
000	C07D 487/04		

BR 9913888 A	January 8, 2002	N/A
000 C07D 487/04		
KR 2001085822 A	September 7, 2001	N/A
000 C07F 009/44		
CN 1326457 A	December 12, 2001	N/A
000 C07D 487/04		
ZA 200102201 A	May 29, 2002	N/A
272 C07D 000/00		
HU 200200355 A2	June 28, 2002	N/A
000 C07D 487/04		
JP 2002527359 W	August 27, 2002	N/A
257 C07D 487/04		
AU 752474 B	September 19, 2002	N/A
000 C07D 487/04		
MX 2001002784 A1	November 1, 2001	N/A
000 A61K 031/505		
SK 200100385 A3	March 4, 2003	N/A
000 C07D 487/04		
US 20030187001 A1	October 2, 2003	N/A
000 A61K 031/519		
NZ 510587 A	November 28, 2003	N/A
000 C07D 487/04		
IN 200100364 P4	March 4, 2005	E
000 C07D 487/04		
EP 1114052 B1	November 16, 2005	E
000 C07D 487/04		
DE 69928414 E	December 22, 2005	N/A
000 C07D 487/04		
ES 2253930 T3	June 1, 2006	N/A
000 C07D 487/04		

DESIGNATED-STATES: AE AL AM AT AU AZ BA BB BG BR BY CA CH CN CR CU CZ
DE DK DM
EE ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR KZ LC LK LR
LS LT LU
LV MD MG MK MN MW MX NO NZ PL PT RO RU SD SE SG SI SK SL TJ TM TR TT
TZ UA UG
US UZ VN YU ZA ZW AT BE CH CY DE DK EA ES FI FR GB GH GM GR IE IT KE
LS LU MC
MW NL OA PT SD SE SL SZ TZ UG ZW AL AT BE CH CY DE DK ES FI FR GB GR
IE IT LI
LT LU LV MC MK NL PT RO SE SI AL AT BE CH CY DE DK ES FI FR GB GR IE
IT LI LT
LU LV MC MK NL PT RO SE SI

APPLICATION-DATA:

PUB-NO	APPL-DESCRIPTOR	APPL-NO
APPL-DATE		
DE 69928414T2	N/A	1999DE-0628414

September 17, 1999		
DE 69928414T2	N/A	1999EP-0969414
September 17, 1999		
DE 69928414T2	N/A	1999WO-US21536
September 17, 1999		
DE 69928414T2	Based on	EP 1114052
N/A		
DE 69928414T2	Based on	WO 200017202
N/A		
WO 200017202A1	N/A	1999WO-US21536
September 17, 1999		
AU 9960475A	N/A	1999AU-0060475
September 17, 1999		
AU 9960475A	Based on	WO 200017202
N/A		
NO 200101357A	N/A	1999WO-US21536
September 17, 1999		
NO 200101357A	N/A	2001NO-0001357
March 16, 2001		
EP 1114052A1	N/A	1999EP-0969414
September 17, 1999		
EP 1114052A1	N/A	1999WO-US21536
September 17, 1999		
EP 1114052A1	Based on	WO 200017202
N/A		
CZ 200100959A3	N/A	1999WO-US21536
September 17, 1999		
CZ 200100959A3	N/A	2001CZ-0000959
September 17, 1999		
CZ 200100959A3	Based on	WO 200017202
N/A		
BR 9913888A	N/A	1999BR-0013888
September 17, 1999		
BR 9913888A	N/A	1999WO-US21536
September 17, 1999		
BR 9913888A	Based on	WO 200017202
N/A		
KR2001085822A	N/A	2001KR-0703527
March 19, 2001		
CN 1326457A	N/A	1999CN-0813218
September 17, 1999		
ZA 200102201A	N/A	2001ZA-0002201
March 16, 2001		
HU 200200355A2	N/A	1999WO-US21536
September 17, 1999		
HU 200200355A2	N/A	2002HU-0000355
September 17, 1999		
HU 200200355A2	Based on	WO 200017202
N/A		
JP2002527359W	N/A	1999WO-US21536

September 17, 1999 JP2002527359W	N/A	2000JP-0574111
September 17, 1999 JP2002527359W	Based on	WO 200017202
N/A		
AU 752474B	N/A	1999AU-0060475
September 17, 1999 AU 752474B	Previous Publ.	AU 9960475
N/A		
AU 752474B	Based on	WO 200017202
N/A		
MX2001002784A1	N/A	2001MX-0002784
March 16, 2001		
SK 200100385A3	N/A	1999WO-US21536
September 17, 1999		
SK 200100385A3	N/A	2001SK-0000385
September 17, 1999		
SK 200100385A3	Based on	WO 200017202
N/A		
US20030187001A1	CIP of	1998US-0042702
March 17, 1998		
US20030187001A1	Provisional	1998US-100954P
September 18, 1998		
US20030187001A1	N/A	1999US-0399083
September 17, 1999		
US20030187001A1	CIP of	US 6001839
N/A		
NZ 510587A	N/A	1999NZ-0510587
September 17, 1999		
NZ 510587A	N/A	1999WO-US21536
September 17, 1999		
NZ 510587A	Based on	WO 200017202
N/A		
IN 200100364P4	N/A	2001IN-CN00364
March 16, 2001		
IN 200100364P4	N/A	1999WO-US21536
N/A		
EP 1114052B1	N/A	1999EP-0969414
September 17, 1999		
EP 1114052B1	N/A	1999WO-US21536
September 17, 1999		
EP 1114052B1	Based on	WO 200017202
N/A		
DE 69928414E	N/A	1999DE-0628414
September 17, 1999		
DE 69928414E	N/A	1999EP-0969414
September 17, 1999		
DE 69928414E	N/A	1999WO-US21536
September 17, 1999		
DE 69928414E	Based on	EP 1114052

N/A

DE 69928414E

Based on

WO 200017202

N/A

ES 2253930T3

N/A

1999EP-0969414

September 17, 1999

ES 2253930T3

Based on

EP 1114052

N/A

200100385 A3 , US 20030187001 A1 , NZ 510587 A

INT-CL (IPC): A61K031/505, A61K031/519 , A61P001/04 , A61P003/10

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A61P019/02 , A61P027/00 , A61P027/06 , A61P029/00 , A61P035/00 ,

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C07D487/02 , C07D487/04 , C07F009/44

ABSTRACTED-PUB-NO: WO 200017202A

BASIC-ABSTRACT:

NOVELTY - 4-Aminopyrrolopyrimidines (I) are new.

DETAILED DESCRIPTION - 4-Aminopyrrolopyrimidines of formula (I) are new.

A = 6-membered aromatic ring or 5 or 6 membered heteroaromatic ring optionally substituted with 1 or more Q;

Q = aliphatic, aryl, heteroaromatic, cycloalkyl, heterocycloalkyl, aralkyl, heteroaralkyl, alkoxycarbonyl, alkyl thioether, alkyl sulfoxide, alkylsulfone, aryl thioether, aryl sulfoxide, aryl sulfone, alkyl carbonyl, aliphatic ether, aromatic ether, carboxamido, alkynyl, alkyl amido, alkyl carboxamido, aryl amido, aryl carboxamido, styryl, aralkyl amido or aralkylcarboxamido (all optionally substituted), halogen, cyano, nitro, NR₄R₅, COOH, OH, CO₂-haloalkyl, C(O)-haloalkyl, tetrazolyl, trifluoromethylsulfonamido, or trifluoromethylcarbonylamino;

L = X, X(O), SO₂, NR, N(C(O)OR), N(C(O)R), N(SO₂R), CH₂X, CH₂NR, CH(NR), CH₂N(C(O)R), CH₂N(C(O)OR), CH₂N(SO₂R), CH(NHR), CH(NHC(O)R), CH(NHSO₂R), CH(NHC(O)OR), CH(OC(O)R), CH(OC(O)NHR), CH=CH, C(=NOR), CH(OR),

$X(O)NR$,
 $N(R)X(O)$, $NRSO_2$, $OC(O)NR$, $NRX(O)NR$, $NRC(O)O$, SO_2NR , $N(C(O)R)S(O)$,
 $N(C(O)R)SO_2$,
 $NRS(O)NR$, $NRSO_2NR$, $X(O)NRC(O)$, $SO_2NRC(O)$, $OS(O)NR$, OSO_2NR , $NRS(O)O$,
 $NRSO_2O$,
 $NRS(O)C(O)$, $NRSO_2C(O)$, $SON(C(O)R)$, $SO_2N(C(O)R)$, $NRSO_2NR$, $C(O)O$,
 $NRP(OR')O$,
 $NRP(OR')$, $NRP(O)(OR')O$, $NRP(O)(OR')$, $N(C(O)R)P(OR')O$, $N(C(O)R)P(OR')$,
 $N(C(O)R)P(O)(OR')O$, $N(C(O)R)P(OR')$, $RbNRSO_2$, $RbNRP(O)$, $RbNRP(O)O$ or a
 group of
 formula (i) - (vi);

$X = O, S$

R, R' = aliphatic, aromatic, heteroaromatic or cycloalkyl groups (all optionally substituted), H or acyl;

Rb = alkylene group, which taken with sulfonamide, phosphonamide or phosphinamide to which it is attached forms a 5 or 6 membered ring fused to A;

R_{85} = together with phosphinamide or phosphonamide is a 5 - 7 membered aromatic, heteroaromatic or heterocyclic ring;

$R_1 = H$, 2-phenyl-1,3-dioxan-5-yl, 1-6C alkyl, 3-8C cycloalkyl, 5-7C cycloalkenyl or optionally substituted phenyl-(1-6C alkyl), the alkyl, cycloalkyl and cycloalkenyl optionally substituted by 1 or more OR_a , provided that OR_a is not located on a C attached to N;

$R_a = H$, 1-6C alkyl or 3-6C cycloalkyl;

$R_2 =$ aliphatic, cycloalkyl, aromatic, heteroaromatic, heterocycloalkyl, aralkyl, heteroaralkyl (all optionally substituted), H, OH, CN, NR_4R_5 or $C(O)NR_4R_5$;

$R_3 =$ cycloalkyl, aromatic, heteroaromatic, heterocycloalkyl (all optionally substituted);

$R_4, R_5 = H$, azabicycloalkyl, optionally substituted alkyl or $Y-Z'$; or

$NR_4R_5 =$ 3 - 7 membered optionally substituted heterocycloalkyl, heterobicycloalkyl or heteroaromatic group;

$Y = C(O)$, $(CH_2)_p$, SO_2 , $C(O)O$, SO_2NH , $C(O)NH$, $(CH_2)_pX$, $(CH_2)_pNH$,

(CH₂)_pS(O) or
(CH₂)_pSO₂;

p, j = 0 - 6; and

Z' = alkyl, amino, aryl, heteroaryl or heterocycloalkyl (all optionally substituted).

provided that when:

L = NRSO₂, NRC(O), NRC(O)O, SO₂NR or OC(O)NR, then R₃ is alkyl, alkenyl or aralkyl (all optionally substituted);

L = CH₂NR, C(O)NR or NRC(O), and R₃ = azacycloalkyl or azaheteroaryl, then j = 0; and

L = O, and R₃ = phenyl, then j = 0.

An INDEPENDENT CLAIM is provided for a method of inhibiting protein kinase activity by administering (I), its salt, prodrug or active metabolite.

ACTIVITY - Cytostatic; vasotropic; immunosuppressive; immunomodulator; antiinflammatory; antiulcer; antibacterial; virucide; anti-HIV; protozoacide; antipsoriatic; osteopathic; nephrotropic; respiratory; hepatotropic; hemostatic; antiasthmatic; gynecological; dermatological; muscular; gastrointestinal; antirheumatic; antiarthritic; neuroprotective; antianemic; ophthalmological; cardiovascular; antiarteriosclerotic; vasotropic; contraceptive.

Female Balb/c mice were treated with pregnant mare's serum gonadotropin, then 2 days later with hCG and the next day with compounds of the invention. Thirty minutes later, animals were injected with 17-estradiol and sacrificed 2-3 hours later. The uterus was removed, weighed, blotted and weighed again to give the fluid content as indicator of inflammation. (I) inhibited the formation of edema (no numerical data).

MECHANISM OF ACTION - Protein Kinase inhibitor; PDGF antagonist; IGF

antagonist; Src inhibitor;

USE - For inhibition of protein kinases, particularly in treatment of angiogenesis, vascular permeability, immune responses or inflammation and specifically for treatment of ulcers, ulcerative colitis, Lyme disease, sepsis, infection by Herpes simplex, Herpes zoster, HIV, parapoxvirus, protozoa or toxoplasmosis, von Hippel Lindau disease, pemphigoid, psoriasis, Paget's disease, polycystic kidney disease, fibrosis, sarcoidosis, cirrhosis, hyperviscosity syndrome, Oster-Weber-Rendu disease, COPD (chronic obstructive pulmonary disease), asthma, exudates, ascites, pleural or pericardial effusions, edema, ovarian hyperstimulation syndrome, pre-eclampsia, menometrorrhagia, endometriosis, chronic inflammation, SLE (not defined), glomerulonephritis, synovitis, IBD (irritable bowel disease), Crohn's disease, rheumatoid and osteo-arthritis, multiple sclerosis, graft rejection, sickle cell anemia, ocular conditions, cardiovascular conditions (e.g. atherosclerosis, restenosis, ischemia, vascular occlusion, venous malformation and carotid obstructive disease), cancer, Crow-Fukase syndrome, diabetic conditions (e.g. glaucoma, diabetic retinopathy or microangiopathy) and to decrease fertility (claimed).

ADVANTAGE - Active against several protein kinases.

CHOSEN-DRAWING: Dwg.0/0

TITLE-TERMS: NEW PYRROLO PYRIMIDINE DERIVATIVE USEFUL TREAT ANGIOGENESIS

VASCULAR PERMEABLE IMMUNE RESPOND INFLAMMATION CANCER
RESPIRATION
DISORDER DECREASE FERTILITY PROTEIN KINASE INHIBIT

DERWENT-CLASS: B02

CPI-CODES: B05-B01J; B06-D08; B14-A01; B14-A02; B14-A02B1; B14-A03;
B14-C03;
B14-C06; B14-C09; B14-C09B; B14-D06; B14-E08; B14-E10;
B14-F01;
B14-F03; B14-F07; B14-F08; B14-G01B; B14-G02; B14-G03;
B14-H01;
B14-H01B; B14-J01; B14-J05; B14-K01; B14-K01A; B14-L06;

B14-N01;

B14-N03; B14-N07; B14-N14; B14-N17; B14-N17C; B14-P01;

B14-S01;

B14-S04;

CHEMICAL-CODES:

Chemical Indexing M2 *01*

Fragmentation Code

C316 D011 D013 D840 G011 G015 G030 G112 G553 H1
H100 H121 H161 H2 H201 H5 H541 H6 H601 H641
H685 H8 K0 K3 K353 M1 M113 M121 M147 M280
M311 M321 M344 M362 M391 M412 M511 M520 M532 M541
M710 M904 M905 P210 P220 P420 P421 P423 P431 P517
P520 P522 P616 P617 P633 P714 P721 P723 P738 P811
P812 P814 P815 P816 P820 P822 P922

Ring Index

01261

Specific Compounds

A1MS7T A1MS7N

Chemical Indexing M2 *02*

Fragmentation Code

C316 D011 D013 D840 G011 G015 G030 G112 G553 H1
H100 H121 H161 H2 H201 H6 H602 H608 H642 K0
K3 K353 M1 M113 M121 M147 M280 M320 M412 M511
M520 M532 M541 M710 M904 M905 P210 P220 P420 P421
P423 P431 P517 P520 P522 P616 P617 P633 P714 P721
P723 P738 P811 P812 P814 P815 P816 P820 P822 P922

Ring Index

01261

Specific Compounds

A1MS8T A1MS8N

Chemical Indexing M2 *03*

Fragmentation Code

C316 D011 D013 D840 G011 G015 G030 G112 G553 H1
H100 H121 H161 H2 H201 H6 H601 H602 H642 K0
K3 K353 M1 M113 M121 M147 M280 M320 M412 M511
M520 M532 M541 M710 M904 M905 P210 P220 P420 P421
P423 P431 P517 P520 P522 P616 P617 P633 P714 P721
P723 P738 P811 P812 P814 P815 P816 P820 P822 P922

Ring Index

01261

Specific Compounds

A1MS9T A1MS9N

Chemical Indexing M2 *04*

Fragmentation Code

C316 D011 D013 D840 G011 G015 G030 G112 G553 H1
H100 H121 H161 H2 H201 H6 H601 H602 H642 K0

K3 K353 M1 M113 M121 M147 M280 M320 M412 M511
M520 M532 M541 M710 M904 M905 P210 P220 P420 P421
P423 P431 P517 P520 P522 P616 P617 P633 P714 P721
P723 P738 P811 P812 P814 P815 P816 P820 P822 P922

Ring Index

01261

Specific Compounds

AlMSAT AlMSAN

Chemical Indexing M2 *05*

Fragmentation Code

C316 D011 D013 D840 G012 G015 G030 G112 G553 H1
H100 H121 H161 H2 H201 H6 H601 H602 H642 K0
K3 K353 M1 M113 M121 M147 M280 M320 M412 M511
M520 M532 M541 M710 M904 M905 P210 P220 P420 P421
P423 P431 P517 P520 P522 P616 P617 P633 P714 P721
P723 P738 P811 P812 P814 P815 P816 P820 P822 P922

Ring Index

01261

Specific Compounds

AlMSBT AlMSBN

Chemical Indexing M2 *06*

Fragmentation Code

C316 D011 D013 D840 G010 G015 G030 G112 G553 H1
H100 H121 H161 H2 H201 H6 H602 H641 K0 K3
K353 M1 M113 M121 M147 M280 M320 M412 M511 M520
M532 M541 M710 M904 M905 P210 P220 P420 P421 P423
P431 P517 P520 P522 P616 P617 P633 P714 P721 P723
P738 P811 P812 P814 P815 P816 P820 P822 P922

Ring Index

01261

Specific Compounds

AlMSCT AlMSCN

Chemical Indexing M2 *07*

Fragmentation Code

C316 D011 D013 D840 G010 G015 G030 G112 G553 H1
H100 H121 H161 H2 H201 H3 H341 K0 K3 K353
M1 M113 M121 M147 M280 M320 M412 M511 M520 M532
M541 M710 M904 M905 P210 P220 P420 P421 P423 P431
P517 P520 P522 P616 P617 P633 P714 P721 P723 P738
P811 P812 P814 P815 P816 P820 P822 P922

Ring Index

01261

Specific Compounds

AlMSDT AlMSDN

Chemical Indexing M2 *08*

Fragmentation Code

D011 D013 D840 G012 G015 G030 G112 G553 H1 H100
 H121 H161 H2 H201 H6 H602 H641 H685 K0 K3
 K353 M1 M113 M121 M147 M280 M311 M321 M344 M353
 M391 M412 M511 M520 M532 M541 M710 M904 M905 P210
 P220 P420 P421 P423 P431 P517 P520 P522 P616 P617
 P633 P714 P721 P723 P738 P811 P812 P814 P815 P816
 P820 P822 P922
 Ring Index
 01261
 Specific Compounds
 A1MSET A1MSEN

Chemical Indexing M2 *09*

Fragmentation Code
 C316 D011 D013 D840 G013 G015 G030 G112 G553 H1
 H100 H121 H161 H2 H201 H6 H602 H608 H642 K0
 K3 K353 M1 M113 M121 M147 M280 M320 M412 M511
 M520 M532 M541 M710 M904 M905 P210 P220 P420 P421
 P423 P431 P517 P520 P522 P616 P617 P633 P714 P721
 P723 P738 P811 P812 P814 P815 P816 P820 P822 P922
 Ring Index
 01261
 Specific Compounds
 A1MSFT A1MSFN

Chemical Indexing M2 *10*

Fragmentation Code
 C316 D011 D013 D840 G011 G015 G030 G112 G553 H1
 H100 H121 H161 H2 H201 H6 H602 H641 K0 K3
 K353 L1 L143 M1 M113 M121 M147 M280 M320 M412
 M511 M520 M532 M541 M710 M904 M905 P210 P220 P420
 P421 P423 P431 P517 P520 P522 P616 P617 P633 P714
 P721 P723 P738 P811 P812 P814 P815 P816 P820 P822
 P922
 Ring Index
 01261
 Specific Compounds
 A1MSGT A1MSGN

Chemical Indexing M2 *11*

Fragmentation Code
 C316 D011 D013 D840 G011 G015 G030 G112 G553 H1
 H100 H121 H161 H2 H201 H3 H341 H6 H601 H641
 K0 K3 K353 M1 M113 M121 M147 M280 M320 M412
 M511 M520 M532 M541 M710 M904 M905 P210 P220 P420
 P421 P423 P431 P517 P520 P522 P616 P617 P633 P714
 P721 P723 P738 P811 P812 P814 P815 P816 P820 P822
 P922
 Ring Index
 01261

Specific Compounds
AlMSHT AlMSHN

Chemical Indexing M2 *12*

Fragmentation Code

C316 D011 D013 D840 G014 G015 G030 G112 G553 H1
H100 H121 H161 H2 H201 H6 H601 H609 H643 K0
K3 K353 M1 M113 M121 M147 M280 M320 M412 M511
M520 M532 M541 M710 M904 M905 P210 P220 P420 P421
P423 P431 P517 P520 P522 P616 P617 P633 P714 P721
P723 P738 P811 P812 P814 P815 P816 P820 P822 P922

Ring Index

01261

Specific Compounds
AlMSIT AlMSIN

Chemical Indexing M2 *13*

Fragmentation Code

C316 D011 D013 D840 G010 G015 G030 G112 G553 H1
H100 H121 H161 H2 H201 H5 H541 H8 K0 K3
K353 M1 M113 M121 M147 M210 M211 M272 M281 M320
M412 M511 M520 M532 M541 M710 M904 M905 P210 P220
P420 P421 P423 P431 P517 P520 P522 P616 P617 P633
P714 P721 P723 P738 P811 P812 P814 P815 P816 P820
P822 P922

Ring Index

01261

Specific Compounds
AlMSJT AlMSJN

Chemical Indexing M2 *14*

Fragmentation Code

C316 M710 M905 P210 P220 P420 P421 P423 P431 P517
P520 P522 P616 P617 P633 P714 P721 P723 P738 P811
P812 P814 P815 P816 P820 P822 P922

Ring Index

01261

Specific Compounds
AlMSKT AlMSKN

Chemical Indexing M2 *15*

Fragmentation Code

C316 D011 D013 D840 G015 G019 G030 G112 G553 H1
H100 H121 H161 H2 H201 H6 H601 H603 H608 H643
K0 K3 K353 M1 M113 M121 M147 M280 M320 M412
M511 M520 M532 M541 M710 M904 M905 P210 P220 P420
P421 P423 P431 P517 P520 P522 P616 P617 P633 P714
P721 P723 P738 P811 P812 P814 P815 P816 P820 P822
P922

Ring Index

01261
Specific Compounds
AlMSLT AlMSLN

Chemical Indexing M2 *16*

Fragmentation Code

C316 D011 D013 D840 G015 G019 G030 G112 G553 H1
H100 H121 H161 H2 H201 H6 H601 H609 H643 K0
K3 K353 M1 M113 M121 M147 M280 M320 M412 M511
M520 M532 M541 M710 M904 M905 P210 P220 P420 P421
P423 P431 P517 P520 P522 P616 P617 P633 P714 P721
P723 P738 P811 P812 P814 P815 P816 P820 P822 P922

Ring Index

01261
Specific Compounds
AlMSMT AlMSMN

Chemical Indexing M2 *17*

Fragmentation Code

G553 H1 H100 H121 H161 H2 H201 H6 H601 H609
H643 K0 K3 K353 M1 M113 M121 M147 M280 M320
M412 M511 M520 M532 M541 M710 M904 M905 P210 P220
P420 P421 P423 P431 P517 P520 P522 P616 P617 P633
P714 P721 P723 P738 P811 P812 P814 P815 P816 P820
P822 P922

Ring Index

01261
Specific Compounds
AlMSNT AlMSNN

Chemical Indexing M2 *18*

Fragmentation Code

C316 D011 D013 D840 G011 G015 G030 G112 G553 H1
H100 H121 H161 H2 H201 H6 H601 H603 H642 K0
K3 K353 M1 M113 M121 M147 M280 M320 M412 M511
M520 M532 M541 M710 M904 M905 P210 P220 P420 P421
P423 P431 P517 P520 P522 P616 P617 P633 P714 P721
P723 P738 P811 P812 P814 P815 P816 P820 P822 P922

Ring Index

01261
Specific Compounds
AlMSOT AlMSON

Chemical Indexing M2 *19*

Fragmentation Code

C316 D011 D013 D840 G014 G015 G030 G112 G553 H1
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K0 K3 K353 M1 M113 M121 M147 M280 M320 M412
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P721 P723 P738 P811 P812 P814 P815 P816 P820 P822
P922
Ring Index
01261
Specific Compounds
A1MSPT A1MSPN

Chemical Indexing M2 *20*

Fragmentation Code
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H100 H121 H161 H2 H201 H6 H601 H602 H609 H643
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P721 P723 P738 P811 P812 P814 P815 P816 P820 P822
P922
Ring Index
01261
Specific Compounds
A1MSQT A1MSQN

Chemical Indexing M2 *21*

Fragmentation Code
B615 B701 B711 B712 B720 B731 B741 B793 B813 B815
B819 B831 B840 C116 C216 C316 D010 D011 D013 D014
D019 D020 D029 D040 D049 D840 F010 F012 F015 F018
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G010 G011 G012 G013 G014 G015 G016 G019 G020 G021
G022 G029 G030 G039 G040 G050 G100 G111 G112 G113
G221 G299 G551 G552 G553 G561 G562 G563 H1 H100
H101 H102 H103 H121 H122 H123 H141 H142 H143 H161
H181 H182 H183 H201 H211 H321 H322 H323 H341 H342
H343 H401 H402 H403 H404 H405 H421 H422 H423 H424
H441 H442 H443 H444 H461 H481 H521 H522 H523 H541
H542 H543 H561 H562 H581 H582 H583 H584 H589 H592
H594 H596 H598 H599 H600 H608 H609 H621 H622 H623
H641 H642 H643 H681 H682 H683 H684 H685 H686 H689
H713 H714 H716 H721 H722 H723 H731 J011 J012 J013
J014 J111 J112 J113 J131 J132 J133 J211 J212 J221
J231 J232 J261 J271 J311 J312 J321 J322 J331 J332
J341 J342 J351 J361 J371 J372 J373 J581 J582 J583
K340 K351 K352 K353 K399 K442 K499 K620 K640 K699
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L462 L463 L499 L520 L532 L550 L560 L599 L640 L699
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M137 M139 M141 M142 M143 M146 M147 M148 M149 M150
M210 M211 M212 M213 M214 M215 M216 M220 M221 M222
M223 M224 M225 M226 M231 M232 M233 M240 M250 M262
M271 M272 M273 M280 M281 M282 M283 M311 M312 M313

M314 M315 M316 M320 M321 M322 M323 M331 M332 M333
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M383 M391 M392 M393 M411 M412 M511 M512 M513 M520
M521 M522 M523 M530 M531 M532 M533 M540 M541 M542
M543 M630 M640 M650 M710 M904 M905 P210 P220 P420
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P721 P723 P738 P811 P812 P814 P815 P816 P820 P822
P922
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00061 00262 01261
Markush Compounds
200015-54801-T 200015-54801-N

SECONDARY-ACC-NO:

CPI Secondary Accession Numbers: C2000-085643